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Stochastic ground-state processes

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Associated with the ground state of a quantum system, there is a unique stochastic process which, in general, has diffusion and jumping components. This is illustrated in two exact models. The drift and the jumping kernel of the ground-state process may be obtained directly without solving the Schrödinger equation. A method is proposed to extract expectation values and Euclidian correlation functions from a numerical simulation of the process. The method applies equally well to boson and fermion systems, without the sign problem.

I. STOCHASTIC PROCESSES AND GROUND-STATE DYNAMICS

The ground state and Euclidian dynamics of a quantum system are uniquely associated with a stochastic process. Let ρ and G be the unique invariant measure density and the generator of stochastic process such that

$$-\hbar\rho^{1/2}G\rho^{-1/2}=H \tag{1.1}$$

is the Hamiltonian operator of a physical system. Then $\rho^{1/2}$ is the (zero energy) ground state, i.e., $H\rho^{1/2}=O$ (Refs. 1 and 2) ($\rho^{1/2}=\phi$). From the representation $T=\exp\{-tG\}$ for the operator semigroup,

$$(T_t f)(x)=\int P(t,x,dy)f(y)\ , \tag{1.2}$$

associated with the transition functions of the Markov process, it follows that Euclidian correlations of the theory (Schwinger functions) are obtained from the stochastic correlations of the process. The stochastic process may therefore be used to study the dynamical properties of the quantum system.

The existence of a process with a unique invariant measure insures the existence of a Schrödinger picture for the quantum system, and stochastic techniques like the theory of small random perturbations by Wentzell and Freidlin,[3,4] may be used to obtain rigorous nonperturbative results, not generally accessible through functional analytic methods.[5,6] The stochastic process involved in this construction is a classical stochastic process which happens to have $\rho=|\phi|^2$ as its invariant measure, and generates a set of Euclidian correlations. However, it should not be confused with the quantum probability[7,8] process associated with real-time quantum evolutions.

This stochastic formulation of quantum systems has, in the past, been used mostly for boson systems. In this paper, we will concentrate on methods which are also appropriate for fermion systems. In the occupation number representation, fermion systems appear to be associated to jump processes which, for boson systems, are characteristic of nonlocal interactions. Because of the formal similarities, we will first review the construction of the stochastic process for nonlocal interactions.[2,9]

Let H be a Hamiltonian operator and $\phi(x)$ its (real) lowest-energy eigenstate (which is adjusted to zero energy by the addition of a constant to H)

$$(H\phi)(x)=-\frac{\hbar^2}{2m}\Delta\phi(x)+U(x)\phi(x)+\int d^n y\ V(x,y)\phi(y)$$
$$=O \tag{1.3}$$

with $V(x,y)$ real finite and $V(x,y)=V(y,x)$.

From (1.1), for the generator of the ground-state process with invariant measure $\rho=\phi^2$, we obtain

$$(Gf)(x)=\left[\frac{\hbar}{m}\frac{\nabla\phi}{\phi}\nabla\right]f+\frac{\hbar}{2m}\Delta f$$
$$-\frac{1}{\hbar}\int d^n y\ \phi^{-1}(x)V(x,y)\phi(y)\{f(y)-f(x)\}\ . \tag{1.4}$$

Now we compare with the general differential Chapman-Kolmogorov equation

$$\partial_t p(xt|zt')=-\nabla\{b(x,t)p(xt|zt')\}$$
$$+\tfrac{1}{2}\sum_{i,j}\frac{\partial^2}{\partial x_i\partial x_j}\{a_{ij}(x,t)p(xt|zt')\}$$
$$+\int d^n y\{W(x|y)p(yt|zt')$$
$$-W(y|x)p(xt|zt')\} \tag{1.5}$$

for which the generator $Gf=\lim_{\Delta t\downarrow 0}[(T_{\Delta t}f-f)]/\Delta t$ is

$$(Gf)(x)=b(x,t)\nabla_x f(x)+\tfrac{1}{2}a_{ij}(x,t)\frac{\partial^2}{\partial x_i\partial x_j}f(x)+\int d^n y\, W(y|x)\{f(y)-f(x)\}\ . \tag{1.6}$$

Comparing Eqs. (1.4) and (1.6) we conclude that the ground-state process associated with the nonlocal Hamiltonian has the drift, diffusion coefficient, and jumping kernel, respectively:

$$b=\frac{\hbar}{m}\frac{\nabla\phi}{\phi}\ , \tag{1.7}$$

$$a_{ij}=\frac{\hbar}{m}\delta_{ij}\ , \tag{1.8}$$

$$W(y|x)=-\frac{1}{\hbar}\phi^{-1}(x)V(x,y)\phi(y)\ . \tag{1.9a}$$

Notice the association, in processes ruled by nonlocal interactions, of diffusion and jumping.[10] This will also be typical of processes involving bosons and fermions (see below).

Likewise, if the state space of a Hamiltonian is spanned by a discrete set $\{|f\rangle\}$ of basis states we see, by analogy with (1.9a), that the jumping process with kernel

$$W(f|f')=-\frac{1}{\hbar}\mathrm{Re}\left\{\frac{1}{\langle f'|\phi\rangle}\langle f'|H|f\rangle\langle f|\phi\rangle\right\} \tag{1.9b}$$

has an invariant density $\rho(f)=|\langle f|\phi\rangle|^2$, as may easily be checked from the stochastic equation

$$\partial_t\rho(f)=\sum_{f'}\{W(f|f')\rho(f')-W(f'|f)\rho(f)\}\ . \tag{1.10}$$

Notice that in this equation the kernel is defined only up to terms const $\delta_{f,f'}$.

In Eqs. (1.7) and (1.9) the drift and the jumping kernel are both functions of the ground-state wave function ϕ, which in general is not known for a given Hamiltonian. It is, however, possible to formulate the dynamical problem in such a way that the drift and jumping kernel are obtained directly without having to solve the equation $H\phi(x)=\lambda_0\phi(x)$ for the lowest eigenvalue λ_0. Let ϕ_0 be some initial state nonorthogonal to the ground state. Then, in the $t\to\infty$ limit, the solution $\phi_t=\exp\{-(1/\hbar)Ht\}\phi_0$ of the Euclidian equation

$$\hbar\partial_t\phi_t(x)=-H\phi_t(x) \tag{1.11}$$

converges to the ground state. That is, $\exp\{(1/\hbar)\lambda_0 t\}\phi_t\to\phi$. Defining

$$b_t=\frac{\hbar}{m}\frac{\nabla\phi_t}{\phi_t},\quad W_t(y|x)=-\frac{1}{\hbar}\phi_t^{-1}(x)V(x,y)\phi_t(y)\ , \tag{1.12}$$

where ϕ_t is a solution of the Euclidian equation (1.11), we obtain evolution equations for b_t and $W_t(y|x)$:

$$\partial_t b_t(x)=\tfrac{1}{2}\nabla b_t^2(x)+\frac{\hbar}{2m}\nabla(\nabla b_t(x))-\frac{1}{m}\nabla U(x)+\frac{\hbar}{m}\nabla_x\int d^n y\, W_t(y|x)\ , \tag{1.13a}$$

$$\partial_t W_t(y|x)=W_t(y|x)\int d^n z\{W_t(z|y)-W_t(z|x)\}+\tfrac{1}{2}W_t(y|x)\left\{2U(x)-\frac{m}{\hbar}b_t^2(x)-\nabla b_t(x)-2U(y)+\frac{m}{\hbar}b_t^2(y)+\nabla b_t(y)\right\}\ . \tag{1.13b}$$

As ϕ_t converges to the ground state, solutions of Eqs. (1.13) converge to the drift and jumping kernels associated with the ground-state process. Therefore, and as far as the ground-state determination is concerned, the iteration of Eqs. (1.13) is equivalent to finding the solution of the Schrödinger equation. In the general case for processes involving diffusion and jumping, these equations may not be easier to handle than the Schrödinger equation itself. However, in the pure jump case, they have a particularly simple form and, in many-body systems with short-range interactions, they provide a simple numerical simulation algorithm. In addition, the fact that one is dealing directly with transition probability kernels and not with amplitudes circumvents the sign problem in numerical simulations (see below).

For the pure jump case associated with the discrete basis representation $\{|f\rangle\}$, one obtains the (Euclidian) evolution equation

$$\partial_t K_t(f|f')=\sum_g K_t(f|f')\{K_t(g|f)-K_t(g|f')\} \tag{1.14}$$

for the quantity

$$K_t(f|f')=-\frac{1}{\hbar}\frac{1}{\langle f'|\phi_t\rangle}\langle f'|H|f\rangle\langle f|\phi_t\rangle\ ,$$

the jumping kernel being

$$W_t(f|f')=\mathrm{Re}K_t(f|f')\ .$$

Starting from an initial W_0, this equation converges in the $t\to\infty$ limit to the jumping kernel of the ground-state process. We may start, for example, from

$$W_0(f|f')=-\frac{1}{\hbar}\mathrm{Re}\langle f|H|f'\rangle\ ,$$

which corresponds to considering the initial ϕ_t as having the same projection on all basis states. Although Eq. (1.14) by itself contains no explicit dynamical information about the interaction potential, it is able to generate the ground-state kernel because under time evolution it preserves all information introduced by the initial condition, namely $\partial_t\{W_t(f'|f)\ W_t(f|f')\}=0$. That is, what

Eq. (1.14) does is simply to balance the transition probabilities to make them consistent with an invariant measure while, at the same time, preserving the information about the Hamiltonian that is supplied by the initial condition.

For a many-body quantum system, because the number of possible states is very large, the Euclidian equations (1.14) become a very large system. If the interactions are short range, a possible solution is to formulate the iteration on a small cluster simulation of the system to obtain an approximation of the ground-state stochastic kernels. These kernels may then be used to obtain correlation functions by simulating the process in a much larger lattice. The simulation of the process uses Eqs. (1.5) and (1.10) or the corresponding stochastic differential equations.

Expectation values of observables for the process X_t defined by Eqs. (1.7)–(1.9) are the quantum expectation values in the ground state:

$$E\{A(X_t)\}=\int A(x)\rho(x)dx$$
$$=\int \phi(x)A(x)\phi(x)dx=(\phi, A\phi)\ . \qquad (1.15)$$

The multitime correlations of the stochastic process are the Euclidian correlations of the quantum system. For example,

$$E\{A(X_t)A(X_0)\}=\int (T_t A)(x)A(x)\rho(x)dx$$
$$=\int \phi^2(x)A(x)(e^{-t/\hbar(\phi^{-1}H\phi)}A)(x)dx$$
$$=(\phi, Ae^{-(t/\hbar)H}A\phi)\ , \qquad (1.16)$$

and similarly for the general n-point correlation function.

Assume that one chooses to compute the stochastic kernels in a basis $\{|f\rangle\}$ that diagonalizes the observable A for which one wishes to obtain the correlation functions. Then the calculation above also shows that, in such an "adapted occupation number basis," there is no essential difference in the procedures to be used for boson or fermion systems. There is therefore a very important difference between the numerical simulation method obtained from the ground-state process, and the quantum Monte Carlo algorithms.[11]

If the initial state ϕ_0 in the Euclidian equation is not orthogonal to the ground state, the quantity

$$\psi_\tau=e^{-\tau H}\phi_0$$

tends to the ground state when $t\to\infty$. In the projector Monte Carlo method, for example,[12] the weights that are used for the statistical sampling are proportional to the wave function ψ_τ. However, we know that for fermions ψ_τ cannot be positive for all configurations. Decompose the wave function into positive and negative energy parts:

$$\psi_\tau=\psi_\tau^+-\psi_\tau^-\ .$$

At low energies both ψ_τ^+ and ψ_τ^- have nonvanishing projections on the "hard-core" bosonic ground state associated with the fermion problem. Hence, at low temperatures, the simulation spends most of the time below the actual energy of the fermionic ground state. These configurations have to be canceled in the partition function sums, hence a minus sign must appear in some of the weights. A similar effect occurs in frustrated spin systems.

By contrast, in algorithms derived from the ground-state processes, one deals with actual transition probability kernels, not with individual terms in a Suzuki-Trotter decomposition of the partition function. Therefore no sign problem should be expected.

II. EXAMPLES

In Sec. III the algorithm for the ground state, described above, is applied to a numerical simulation of the Hubbard model. Here we will consider two examples where the ground state may explicitly be represented as a functional of the operators of the theory. The study of the examples clarifies the nature of the stochastic processes associated with the ground state. The first example is the BCS model. The BCS ground state

$$|\phi\rangle=\prod_{k,\sigma}(u_k+v_k b_{k\sigma}^\dagger b_{-k,-\sigma}^\dagger)|O\rangle\ ,\quad u_k^2+v_k^2=1 \qquad (2.1)$$

is a zero-energy eigenstate of the Hamiltonian

$$H=\sum_{k,\sigma}E_k u_k^2(b_{k\sigma}^\dagger-\alpha_k b_{-k,-\sigma})(b_{k\sigma}-\alpha_k b_{-k,-\sigma}^\dagger)\ , \qquad (2.2)$$

with

$$\alpha_k=-\alpha_{-k}=\frac{v_k}{u_k}\ . \qquad (2.3)$$

Let $\{|c_{k\sigma}\rangle=b_{k\sigma}^\dagger b_{-k,-\sigma}^\dagger|O\rangle;\ k_i>0\}$ be a basis of Cooper pairs. Then from (1.9b) the ground-state process is a jumping process with kernel

$$W(\{c_{k\sigma}\}|\{c_{k'\sigma'}\})=\frac{\prod_{q\in\{c_{k\sigma}\}}v_q}{\prod_{q\in\{c_{k'\sigma'}\}}v_q}\left\{-\sum_{q\in\{c_{k\sigma}\}}2\sqrt{E_q^2-\Delta_q^2}\,\delta_{\{c_{k\sigma}\},\{c_{k'\sigma'}\}}+\Delta_p\delta_{\{c_{k'\sigma'}\},\{c_{k\sigma}\}+c_p}+\Delta_p\delta_{\{c_{k'\sigma'}\},\{c_{k\sigma}\}-c_p}\right\}\frac{1}{\hbar}\ , \qquad (2.4)$$

with $\Delta_p=2E_p u_p v_p$. $\{c_{k_\sigma}\}$ denotes a set of occupied Cooper pairs, and $\{c_{k\sigma}\}\pm c_p$ is the same set with one more or one less occupied pair. Equation (2.4) is obtained from (1.9b) neglecting a term of the type $\text{const}\delta_{\{c_{k\sigma}\},\{c_{k'\sigma'}\}}$.

Another formulation of the ground-state process which is at least of formal interest is obtained using a representation of the creation and annihilation operators in Grassman variables η_k^*. The representation is

$$b^{\dagger}_{k\sigma}\rightarrow\eta^{*}_{k\sigma},\quad b_{k,\sigma}\rightarrow\left[\frac{d}{d\eta^{*}_{k\sigma}}\right]_{L}, \tag{2.5}$$

where

$$\eta_{k\sigma}\eta^{*}_{q\sigma'}+\eta^{*}_{q\sigma'}\eta_{k\sigma}=\eta^{*}_{k\sigma}\eta^{*}_{q\sigma'}+\eta^{*}_{q\sigma'}\eta^{*}_{k\sigma}=0\ ,$$

and the subscript L in the differentiation symbol means that the variable $\eta^{*}_{k\sigma}$ in a monomial must be pushed to the extreme left before the differentiation is applied.

The representation (2.5) acts on functions of $\{\eta^{*}_{k\sigma}\}$ alone. In this representation the BCS ground state is

$$\phi(\eta^{*})=\prod_{\substack{k,\sigma\\(k_i>0)}}(u_k+v_k\eta^{*}_{k\sigma}\eta^{*}_{-k-\sigma})\ , \tag{2.6}$$

and the Hamiltonian is

$$H=\sum_{k,\sigma}E_k u_k^2\left[\eta^{*}_{k\sigma}-\alpha_k\frac{d}{d\eta^{*}_{-k-\sigma}}\right]\left[\frac{d}{d\eta^{*}_{k\sigma}}-\alpha_k\eta^{*}_{-k-\sigma}\right]\ . \tag{2.7}$$

Performing the transformation induced by $\phi(\eta^{*})$ on H one obtains

$$-\phi^{-1}H\phi=\sum_{k,\sigma}E_k u_k\frac{d}{d\eta^{*}_{-k-\sigma}}\frac{d}{d\eta^{*}_{k\sigma}}-\sum_{k,\sigma}E_k\eta^{*}_{k\sigma}\frac{d}{d\eta^{*}_{k\sigma}}\ . \tag{2.8}$$

Comparing with the standard form of the elliptic operator,

$$\tfrac{1}{2}\sum_{i,j}\alpha_{ij}(x,t)\frac{\partial^2}{\partial x_i\partial x_j}+\sum_i\beta_i\frac{\partial}{\partial x_i}$$

the generator of a diffusion process, one concludes that the BCS ground-state process may formally be interpreted as a diffusion process in Grassman variables, with drift

$$\beta_{k\sigma}=-E_kE_k\eta^{*}_{k\sigma} \tag{2.9a}$$

and diffusion coefficient

$$\alpha_{k\sigma,p\sigma'}=2E_ku_k\delta_{k,-p}\delta_{\sigma,\sigma'}\ . \tag{2.9b}$$

For practical purposes, however, the formulation of the ground state as a jump process in an occupation number basis is probably more useful.

For the second example, consider a supersymmetric hopping model defined on a two-dimensional square lattice by

$$H=\tfrac{1}{2}\sum_{(ij)}\left[-\hbar^2\frac{\partial^2}{\partial\phi_{(ij)}\partial\phi_{(ij)}}+\frac{\partial W}{\partial\phi_{(ij)}}\frac{\partial W}{\partial\phi_{(ij)}}\right]+\tfrac{1}{2}\hbar\sum_{(ij)(kl)}\frac{\partial^2 W}{\partial\phi_{(ij)}\partial\phi_{(kl)}}[c^{\dagger}_{(ij)},c_{(kl)}]\ , \tag{2.10}$$

where $\phi_{(ij)}$ and $c_{(ij)}$ are bosonic and fermionic fields at the lattice point (ij), satisfying

$$\left[\phi_{(ij)},\frac{\hbar}{i}\frac{\partial}{\partial\phi_{(ij)}}\right]=i\hbar\delta_{(ij),(kl)}\ ,\qquad \{c^{\dagger}_{(kl)},c_{(ij)}\}=\delta_{(ij),(kl)}\ . \tag{2.11}$$

For the superpotential $W(\phi)$,

$$W(\phi)=-\frac{t}{\hbar}\sum_{[(ij),(kl)]}\phi_{(ij)}\phi_{(kl)}\ , \tag{2.12}$$

with $[(ij),(kl)]$ denoting a sum over nearest neighbors, the Hamiltonian becomes

$$H=\tfrac{1}{2}\sum_{(ij)}\left[-\hbar^2\frac{\partial^2}{\partial\phi_{(ij)}\partial\phi_{(ij)}}+\left[\sum_{[(kl),(ij)]}\phi_{(kl)}\right]^2\right]-\frac{t}{2}\sum_{[(ij)(kl)]}[c^{\dagger}_{(ij)},c_{(kl)}]\ . \tag{2.13}$$

Denote by $|0\rangle$ and $|-\rangle$ the empty and filled sectors in the fermion Fock space. Then the state

$$|\psi\rangle=e^{W(\phi)/\hbar}\sum_{(ij)}(-1)^{i+j}c_{(ij)}|-\rangle \tag{2.14}$$

is the ground state in the one-hole sector, and is a zero-energy eigenstate of the operator $\bar{H}=H+4t$. Computing the drift and the jumping kernel from Eqs. (1.7) and (1.9), we obtain

$$b_{(ij)}=-\frac{t}{\hbar m}\sum_{[(kl),(ij)]}\phi_{(kl)}\ , \tag{2.15a}$$

$$W(\phi ij|\phi' kl)=-\frac{t}{\hbar}\delta_{[(kl),(ij)]}\delta_{\phi,\phi'}\ . \tag{2.15b}$$

The sum in $b_{(ij)}$ is over all lattice points (kl) that are nearest neighbors to (ij), and $\delta_{[(kl),(ij)]}$ vanishes unless (ij) and (kl) are nearest neighbors. The jumping kernel is computed in the basis

$$|\phi ij\rangle=|\phi\rangle c_{(ij)}|-\rangle\ .$$

We see that the boson-fermion nature of the problem implies that the corresponding process involves both diffusion and jumping.

III. NUMERICAL SIMULATION OF THE GROUND-STATE PROCESS. THE HUBBARD MODEL

As we explained in Sec. I the essential step is the calculation of the jumping kernels $W(f'|f)$ from the asymptotic solution of Eq. (1.14). Notice that $|f\rangle$ runs over all states of the system and therefore, for a system with a large number of degrees of freedom, Eq. (1.14) becomes a differential equation of very high dimension. However, in a system like the Hubbard model,[13] where the elementary interactions are short range, the kernels may, to a good approximation, be obtained by solving the equation for a small cluster, and then storing the solution in a look-up table that is used in a much larger lattice to extract the global properties of the ground state. Notice that the small cluster does not even have to be very small because, for each set of parameters, Eq. (1.14) has to be solved only once.

The Hubbard model is a simple model for interacting electrons in narrow bands. Its current popularity traces its origin to the role played by electron correlations in

high-temperature superconductors. It has been extensively used as a standard test for quantum Monte Carlo methods[11] and this is one of the reasons why we too have used it to test our ground-state process algorithm. Consider then the Hubbard model. The Hamiltonian is

$$H=-t\sum_{\{i,j\}}c^{\dagger}(i)c(j)+U\sum_{i}n_{\uparrow}(i)n_{\downarrow}(i)\ .$$

With $W_0(f'|f)=-\mathrm{Re}\langle f'|H|f\rangle$, the initial values for Eq. (1.14) are

$$W_0(f'|f)=UN_p\ ,\quad f'=f\ ,$$

$$W_0(f'|f)=-t\ \text{ if } f' \text{ differs from } f \text{ by an electron jump to a neighboring site}\ ,$$

$$W_0(f'|f)=0\ \text{ for all other pairs } f,f'\ ,$$

and from the (Euclidian) evolution equation (1.14) the only nonzero W's are those which are nonzero for the initial condition. Therefore, in this case, a 3×3 lattice with periodic boundary conditions already provides an unbiased environment for the elementary jumps. However a 3×3 lattice already carries 4^9 possible different configurations, considering at each site no electron, one electron ($\uparrow$ or $\downarrow$), or a pair of electrons. Using symmetry properties these configurations may be grouped into classes, a class being defined as configurations that can be transformed into one another by translations, rotations, or mirror reflections. This finally leads to 4480 different classes which are classified in Table I according to the number of up and down electrons.

We may therefore limit ourselves to a study of a representative element in each class and their neighboring configurations. The system of equations corresponding to possible, and topologically distinct, transitions between different classes is now solved numerically, and the $W(f'|f)$'s corresponding to its (rapidly) convergent large time solution are stored in a look-up table. Look-up tables were generated for several U/t values in the range 0–10.

Two remarks should be made concerning the calculation of the jumping kernels. The ground-state stochastic equations in Sec. I are derived under the assumption that the energy of the ground state is normalized to zero. Because the ground-state energy is in general not known, it means that the diagonal kernels $W(f'|f)$ are defined only up to an additive constant. This has no effect in the evolution of Eq. (1.14) because the additive constant cancels in the sum of the right-hand side, but it means that the diagonal element values stored in the look-up table are not the actual $W(f|f)$'s. The way to obtain actual values for the stochastic evolution in the ground-state process is through

$$W(f|f)=1-\sum_{g\neq f}W(g|f)\Delta t\ ,$$

provided Δt is sufficiently small compared with the $W(g|f)$'s.

To obtain the properties of the ground state, the simulation starts from a lattice with a certain number of up and down electrons, and the evolution of the stochastic ground-state process is carried out by picking a site at random each time and having its 3×3 neighborhood evolve according to the jumping kernels of the look-up table. In practice all compatible W's are piled up according to their sizes as intervals in the line, and the decision is taken by a random number uniformly distributed in the interval $[0,\sum W]$.

We now present some results of a study of pairing and short-range antiferromagnetic correlations in the ground state of the Hubbard model. More extensive results for this and other modified models are presented elsewhere.[14] The simulations were carried out in a 20×20 lattice with 198 up electrons and 198 down electrons. The boundary conditions are periodic, and the parameter values explored were $U/t=0$, 1, 4, and 10. The initial electron distribution is random (constrained by the Pauli principle). For each case the results we present correspond to 10^6 productive evolutions (i.e., evolutions where there was an actual change in the lattice configuration). Measures of average values are taken only after the number of double occupancies is stabilized. The following quantities were measured: (i) number of doubly occupied sites; (ii) number of hole pairs; (iii) short-range antiferromagnetic correlation; and (iv) medium-range antiferromagnetic correlation. The antiferromagnetic correlation is measured by looking at a neighborhood of each point and counting $+1$ for the antiferromagnetically correlated neighbors, -1 for the ferromagnetic ones, and zero for those that are either empty or have double occupancy. For the "short range" we consider a 3×3 neighborhood and for the "medium range" a 5×5 neighborhood. The results are shown in Table II.

TABLE I. Independent configuration classes in a 3×3 lattice, classified according to the number of up and down electrons.

		Number of electrons ↑									
		0	1	2	3	4	5	6	7	8	9
	0	1	1	2	4	5	5	4	2	1	1
	1	1	3	8	16	23	23	16	8	3	1
	2	2	8	26	54	78	78	54	26	8	2
Number of	3	4	16	54	118	170	170	118	54	16	4
electrons	4	5	23	78	170	250	250	170	78	23	5
↓	5	5	23	78	170	250	250	170	78	23	5
	6	4	16	54	118	170	170	118	54	16	4
	7	2	8	26	54	78	78	54	26	8	2
	8	1	3	8	16	23	23	16	8	3	1
	9	1	1	2	4	5	5	4	2	1	1

TABLE II. Number of doubly occupied sites, hole pairs, and short- and medium-range antiferromagnetic correlations in a 20×20 lattice, for several U/t values.

	U/t			
	0	1	4	10
Double occupancy	99	93	74	50
Hole pairs	54	46	28	14
Short-range antiferr.	53	84	92	117
Medium-range antiferr.	33	75	76	32

TABLE III. Comparison of the average distribution of holes in the Hubbard ground-state simulation (at $U/t=4$), with a purely random distribution for the same total number of holes.

Number of holes in the cluster	Hubbard model	Random distribution
1	37.61	32.97
2	9.19	8.11
3	3.51	3.44
4	1.75	1.54
5	0.67	0.72
6	0.46	0.35
7	0.32	0.17
8	0.13	0.09
9	0.12	0.04
10	0.03	0.02
11	0.08	0.01
12	0.03	0.00

A critical issue in models of high-temperature superconductivity is whether or not the effect is due to a type of Bose condensation of preexisting local pairs of carriers. In particular, the short coherence lengths observed seem to favor such a local pair picture. It is therefore important to search for any symptoms of dynamical hole pairing in the Hubbard model. One sees from Table II that the number of hole pairs decreases with U/t, but that is to be expected from the statistical effect of the decreasing double occupancy which also decreases the number of holes. To disentangle the statistics from dynamical effects we compare, in Table III, the average distribution of holes in the Hubbard model ground state (at $U/t=4$) with a purely random distribution for the same total number of holes. The first column defines the size of the hole clusters, and the second and the third columns contain the average number of such clusters in the Hubbard model and in a random distribution. The conclusion is that there is no essential distinction between the random unbiased distribution of holes and the Hubbard model. Therefore we find no evidence for hole-pair formation in the Hubbard model. Incidentally, this agrees with the analytical estimates of Ref. 15, where it was concluded that the Hubbard model by itself does not lead to pair formation, and that an additional pairing interaction seems to be needed in models of high-T_c superconductivity.

What our results show is evidence of short-range antiferromagnetic correlation, although already at a modest medium range the correlation seems to be lost.

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[10]In the modelization of quantum systems, there are potentials that supply the simplest examples for each type of physical behavior. For example, the harmonic oscillator is typical of a pure point spectrum, the Coulomb potential typical of systems with both point and continuous spectra and accumulation of levels at the ionization threshold, etc. For roton excitations the nonlocal convolution potentials (Ref. 9), of which the simplest one is the symmetric translation potential $(V\psi)(x)=\lambda\psi(x+a)+\lambda^*\psi(x-a)$, provide perhaps the simplest model. In the stochastic interpretation of the Euclidian process the roton is the situation where slow forward diffusion and backward jumps exactly compensate for one another. This may be considered a rigorous formulation of an old image of Feynman, according to which one type of roton excitation may be viewed as a group of children going down a slide, then going around and coming back to the slide again.

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